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# Electronic structure of Ge–Si superlattices grown on Ge (001)

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**Abstract.** We have studied the electronic energy structure of pseudomorphic $Ge_m/Si_n$ superlattices by using the empirical tight-binding method. Effects of the band offset, sublattice periodicity and the lateral lattice constant on the transition energies have been investigated. We found that $Ge_m/Si_n$ superlattices grown on Ge (001) can have a direct band gap, if $m + n = 10$ and $m = 6$. However, optical matrix elements for in-plane and perpendicular polarized light are negligible for the transition from the highest valence band to the lowest conduction band state at the centre of the superlattice Brillouin zone.

The novel properties discovered in the electron systems of lower dimensionality have created a major impact in solid state electronics leading to new concepts in electronic devices. In this context, it is hoped that pseudomorphic Si–Ge superlattices can compensate for the shortcomings of silicon and can open new horizons in the applications of Si-based devices in photonics. In an effort to fabricate a high carrier mobility direct-band semiconductor, the Si–Ge superlattices grown on the (001) substrate have been the focus of attention [1, 2]. While the electroreflectance measurements of $Si_4/Ge_4$ grown on Si (001) have indicated new optical transition [1], theoretical studies [3–6] showed that the difference between the direct and indirect band gap, $\delta E = E_{g,i} - E_{g,d}$, decreases with increasing $n$, but the gap is still indirect. For example, it was found [3, 4] that $\delta E$ is as small as 0.07 eV for the largest superlattice periodicity ($2n = 12$) one can obtain for $Si_n/Ge_n$ grown on Si (001). Moreover, optical matrix elements of the transition to the lowest zone folded states were found to be small [7].

In view of evidence indicating that the strained $Si_n/Ge_n$ laterally restricted to Si (001) has an indirect band gap, attention has been drawn to the Si–Ge superlattices with different structural parameters [8, 9]. In fact, as argued earlier a pseudomorphic superlattice represented by $\{Si_{1-x}Ge_x\}_{n,a_\parallel}/\{Si_{1-y}Ge_y\}_{m,a_\parallel}$ provides several degrees of freedom for controlling the electronic properties. For example, in the superlattice with $x = 0$ and $y = 1$ the lateral lattice constant $a_\parallel$ and the superlattice periodicity, $n + m$, (also $n$ and $m$ itself) are important parameters for controlling the electronic structure. Since the lateral lattice constant of a substrate $Si_{1-z}Ge_z(001)$ can vary between $a_\parallel^{Si}$ (equilibrium lattice constant of Si, i.e. 5.43 Å/$\sqrt{2}$) and $a_\parallel^{Ge}$, the sublattices grown in registry with this substrate undergo a lateral compressive (expansive) strain, while the lattice constant in the perpendicular direction expands (contracts). This gives rise to a uniform tetragonal distortion if the misfit dislocations are prevented from forming.

In this paper we first investigate the effect of the structural parameters on the direct and indirect band gaps of the pseudomorphic Si–Ge superlattices. Guided by these findings and based on the electronic structure calculations, which were performed for several supercells by using the empirical tight-binding method, we determine the structural parameters which make the band gap direct.

It is known that Si–Ge superlattices generally make type-II band alingments, such that the edge of the conduction band and the top of the valance band occur in the Si and Ge sublattices, respectively. To examine the lowest conduction band states of the $Si_n/Ge_n$ we concentrate on the Si-sublattice. The minima of the conduction band of bulk Si occur along the six equivalent [001] directions. These directions are labelled as $\Delta$ in the (fcc) Brillouin zone (BZ) of the bulk Si. In the superlattice grown on the (001) plane, four $\Delta$ directions, which are labelled by $\Delta_\parallel$ coincide with the $\Gamma M$ direction of the superlattice BZ (see inset of figure 1). The remaining two are along the superlattice direction [001] and are labelled by $\Delta_\perp$. Bands along $\Delta_\perp$ are folded. In the absence of strain in the Si-sublattice the minimum of the lowest conduction band state along the $\Gamma M$ direction of the SBZ occurs at relatively lower energy than the lowest folded states along the $\Gamma Z$ direction. Moreover, the lowest conduction band state was found to be itinerant [3, 6]. This is the situation for the strained $Si_n/Ge_n$ ($n \leq 6$) superlattices grown on the Si (001). If, however, a tetragonal strain is induced by forcing the Si sublattice to have $a_\parallel > a_\parallel^{Si}$ the bands along $\Delta_\parallel$ and $\Delta_\perp$ are expected to experience different shifts.

We explored this situation by examining the bands of Si and Ge supercells under tetragonal strain. The variation of

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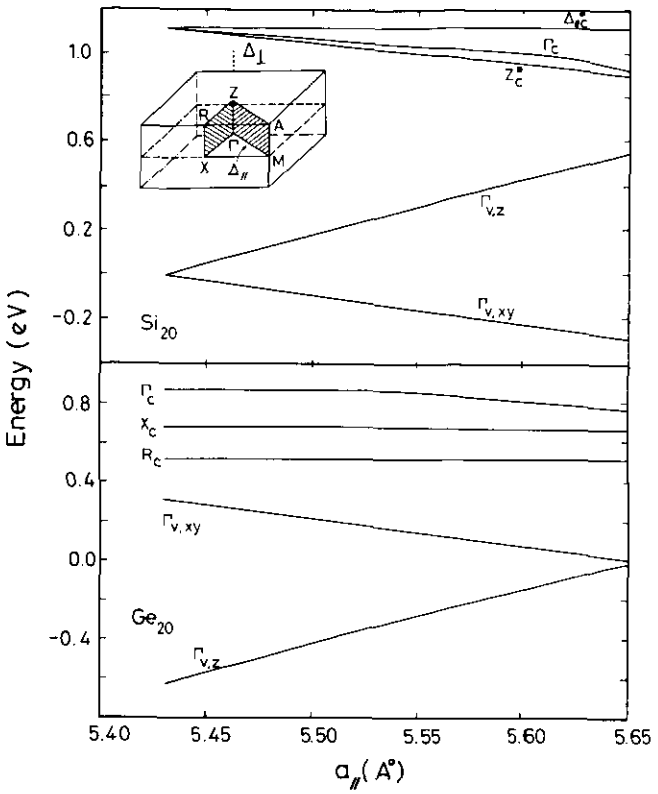


**Figure 1.** Variation of the energy of the lowest conduction band states ($Z_c^*$, $\Delta_{\|c}^*$ along ΓZ and ΓM directions) and $\Gamma_c$ state and highest valance band states ($\Gamma_{v,z}$ and $\Gamma_{v,xy}$) of $Si_{20}$ and $Ge_{20}$ supercells as a function of the lateral lattice constant $a_{\|}$. The symmetry points and directions of the superlattice Brillouin zone are shown in the inset.

the lowest conduction and highest valance bands of $Si_m$ and $Ge_m$ superlattices are calculated as a function of $a_{\|}$. Our results are presented in figure 1 for $m = 20$. In these calculations the perpendicular lattice parameter $a_\perp$ corresponding to a given $a_{\|}$ are calculated by using elastic constants. Earlier it was shown that $a_\perp$ obtained from the Poisson ratio is in compliance with that obtained by using *ab initio* calculations [10]. The results of the fully optimized structure calculations on the Si–Ge superlattices show that in general $a_\perp$ differs slightly from the value obtained by using the Poisson ratio. Moreover, interlayer spacings in the sublattices are *not homogeneous* [3, 4]. Nevertheless, in view of the accuracy obtainable from the empirical tight-binding calculations the structural parameters obtained from the elastic constants suite to the objectives of our calculation. The energy parameters given by Li and Chung [11] are scaled [12] by $d^{-\eta}$ with the scaling exponent $\eta = 2$ when the interatomic distances of the sublattices deviate from their equilibrium values in the presence of the strain. Since splitting of the top of the valence band state at the point, $\delta E_{001}$, is related to the deformation potential $b$, and strain components $\epsilon_{xx}$ and $\epsilon_{zz}$ as $\delta E_{001} = 2b(\epsilon_{zz} - \epsilon_{xx})$, the exponent $\eta$ can be fitted to the deformation potential. Expressing the deformation potential [13] in terms of the strain components, first and second nearest-neighbour tight-binding energy parameters and $\eta$, we find $\eta \sim 1.8$. This justifies the value of exponent $\eta = 2$ used earlier in several calculations. For $Si_{20}$ in figure 1 the lowest conduction band state $Z^*$ along the ΓZ direction and the minimum $\Delta_{\|}^*$ of the lowest conduction band along $\Delta_{\|}$ are both lowered as $a_{\|} \rightarrow a_{\|}^{Ge}$. Moreover, the state $Z^*$ is lowered below the $\Delta_{\|}^*$ state, and the energy difference $E_{\Delta_{\|}^*} - E_{Z^*}$ increases with increasing $a_{\|} - a_{\|}^{Si}$. We note that the $Z^*$ state corresponds to the minimum $\Delta_\perp^*$ of the lowest conduction band along $\Delta_\perp$, which is folded to ΓZ upon the superlattice formation. Similary, the splitting of the valance bands increases as $a_{\|} \rightarrow a_{\|}^{Ge}$, so that the $p_z$-like state raises towards $Z^*$, but $p_{xy}$ states are lowered.

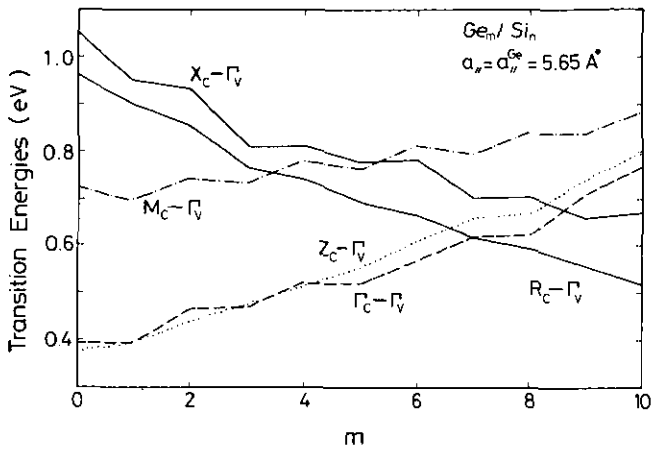


**Figure 2.** Variation of the relevant transition energies of $Ge_m/Si_n$ with the number of the Ge layers $m$. The superlattice is laterally restricted to the Ge (001) surface so that $a_{\|} = a_{\|}^{Ge}$ and $m + n = 20$. ($\Delta E_v = 0.31$ eV).

In view of the above discussion one concludes that the lowest conduction band state, $\Delta_\perp^*$, can be folded to the centre of superlattice BZ to yield a direct band gap for a pseudomorphic $Ge_m/Si_n$ superlattice grown on Ge (001). This can be achieved for certain superlattice periodicity. For example, if the lowest conduction band state $\Delta_\perp^*$ were occured exactly at $k_x = 0, k_y = 0$, and $k_z = 8\pi/5a$ for a strain-free $Si_l$ superlattice, this state $\Delta_\perp^*$ would fold to Γ for $l = 20$ (which has $G_3 = 2\pi/5a$ for the magnitude of the shortest reciprocal vector). For a strained $Ge_m/Si_n$ superlattice grown on Ge (001) $\Delta_\perp^*$ does not appear exactly at $k_z = 8\pi/5a$. However, small deviations from the value $8\pi/5a$ can accounted by varying lattice strain and sublattice periodicity but by keeping $2(m + n) = 20$ so that the minimum value $\Delta_\perp^*$ may occur at Γ point upon folding. Figure 2 shows the variation of various transition energies as a function of $m$ for the strained $Ge_m/Si_n$ superlattice grown on Ge (001). For $5 \leq m \leq 6$ the lowest conduction band state occurs at Γ, attributing directness to the band. The superlattice with $m = 7$ lies at the borderline and beyond $m = 7$ the Ge character dominates and thus the lowest conduction band state at R dips below that at Γ. For $m < 5$ the lowest conduction band state starts to occur either at Z or along ΓZ. These results are in agreement with the band structure of $Ge_m/Si_n$ which are calculated by using the self-consistent pseudopotential calculation [9] as well as experiment [2]. Note that the calculated transition energies as a function of the number of the Ge

layers in the $Ge_m/Si_n$ superlattice is not continuous, but display wiggles in figure 2. This is due to the discrete variation of $m$, which leads to discrete changes in the geometrical parameters and hence to the discontinuous variation in (folded) band energies.

We note that the transition energies in figure 2 are obtained from the band structure calculations of the $Ge_m/Si_n$ superlattice. Because of the emprical nature of the method the elements of the Hamiltonian matrix (i.e. self-energies and hopping energies) are inputs in our calculations. In this context, the value of the band offset is implemented in our calculations by upshifting the self-energies (or the diagonal elements of the Hamiltonian matrix) of the Ge orbitals by $\Delta E_v$. The value of the band offset we used in our calculations was obtained from the earlier *ab initio* calculations [10]. Since the band offset is the crucial parameter which influences the conduction band structure of the superlattice, we investigated whether the value of $\Delta E_v$ affects our conclusions regarding the directness of the band gap. In figure 3 we present the variation of the transition energies as a function of $\Delta E_v$ calculated for $Ge_6/Si_4$ and $Ge_7/Si_3$ both having $a_{\parallel} = a_{\parallel}^{Ge}$. The band gap of $Ge_6/Si_4$ is direct as long as $\Delta E_v \leq 1$ eV, but the difference between the direct and indirect gap decreases as $\Delta E_v$ increases. In contrast, the directness of the band gap of $Ge_7/Si_3$ is sensitive to the value of the band offset. For example, the $R_c$–$\Gamma_v$ transition energy becomes smaller than the lowest direct transition energy and thus the gap becomes indirect if $\Delta E_v \leq 0.3$ eV. Note that the band offset $\Delta E_v$ is affected due to the upshifting of the maximum valance band state by the one-third of the spin–orbit coupling energy $\Delta_0$. The value of $\Delta_0$ is negligible for Si ($\Delta_0 = 0.04$ eV) but significant for Ge ($\Delta_0 = 0.3$ eV). Consequently, owing to the spin–orbit coupling $\Delta E_v$ is increased by 0.1 eV for a Ge/Si superlattice [10]. The transition energies illustrated in figure 2 are calculated by $\Delta E_v$ which does not include the spin–orbit coupling. As a matter of fact, this effect is neglected in several studies of Si/Ge superlattices. However, this effect is implicit in the discussion of figure 3 in which $\Delta E_v$ is taken as a parameter.

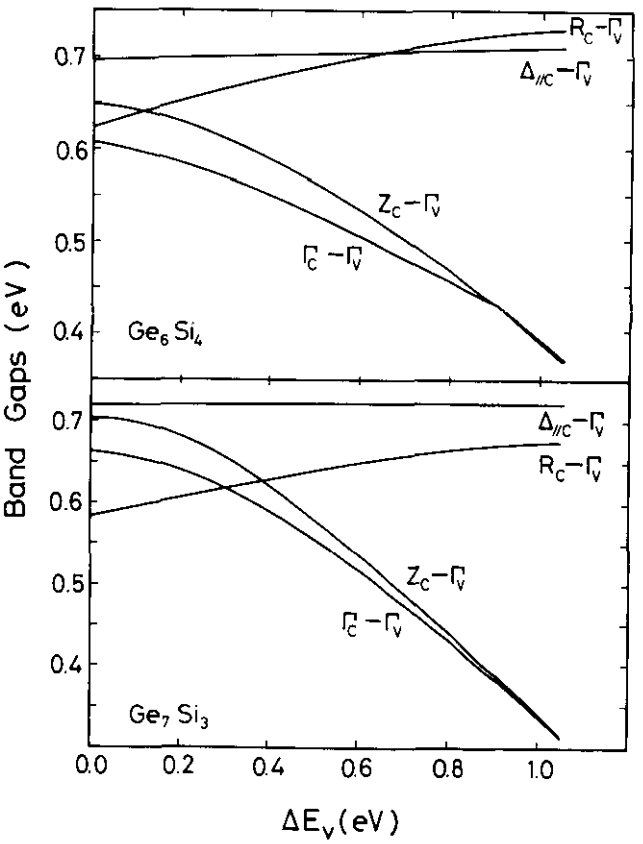


**Figure 3.** Variation of the transition energies with respect to the band offset, $\Delta E_v$ for (top) $Ge_6/Si_4$ and (bottom) $Ge_7/Si_3$. Superlattices are restricted to the Ge (001).

**Table 1.** Calculated optical transition energies (eV) from $p$th highest valence band state to the $q$th lowest conduction band state (i.e. $E_{vp} \longrightarrow E_{cq}$) at the zone centre. All optical matrix elements for the in-plane (||) and perpendicular (⊥) light polarization are negligible, except those indicated by stars have small but finite values ($\sim 10^{-2}$ in au). ($\Delta E_v = 0.31$ eV).

| | $Ge_6Si_4$/Ge (001) | | | $Ge_7Si_3$/Ge (001) | | |
|---|---|---|---|---|---|---|
| | Energy | \|\| Pol. | ⊥ Pol. | Energy | \|\| Pol. | ⊥ Pol. |
| $E_{c1} - E_{v1}$ | 0.57 | | | 0.62 | | |
| $E_{c1} - E_{v2}$ | 0.87 | | | 0.84 | * | |
| $E_{c1} - E_{v3}$ | 0.89 | | | 0.85 | * | |
| $E_{c2} - E_{v1}$ | 0.63 | | * | 0.66 | | * |
| $E_{c2} - E_{v2}$ | 0.93 | * | | 0.88 | | |
| $E_{c2} - E_{v3}$ | 0.95 | * | | 0.89 | | |

From the above discussion it becomes clear that $Ge_6/Si_4$ grown on Ge (001) is a direct band gap semiconductor. However, the directness of the band gap can have important technological implications only if the lowest direct transitions are allowed and the value of the related transition matrix elements are subtantial. To this end we calculate optical matrix elements for in-plane and perpendicular polarizations for direct transitions at $\Gamma$. In the emprical tight-binding method the optical matrix element can be approximated [14] by

$$T_{nk \to n'k'} \propto \Big| \sum_{\alpha'\nu'\alpha\nu} C^{n'*}_{\alpha'\nu'}(k) C^{n}_{\alpha\nu}(k) \times \sum_{l} \exp i\boldsymbol{k}\cdot(\boldsymbol{R}_l + \boldsymbol{\tau}_{\nu\nu'}) E^{l\nu\nu'}_{\alpha\alpha'} \hat{\boldsymbol{\epsilon}}\cdot(\boldsymbol{R}_l + \boldsymbol{\tau}_{\nu\nu'}) \Big|^2 \tag{1}$$

where $C^{n}_{\alpha\nu}(k)$ is the coefficient of the Bloch sum, $R_l$ is the Bravais lattice vector and $\tau_{\nu\nu'}$ is the distance between the nuclei, $\nu$ and $\nu'$, $\alpha$ labels the atomic orbitals. The energy integral, $E^{l\nu\nu'}_{\alpha\alpha'} = \langle \phi_\alpha(r)|H|\phi_{\alpha'}(r - R_l - \tau_{\nu\nu'})\rangle$, corresponds to the energy parameter in our calculation, and $\hat{\epsilon}$ is the polarization vector of the light. The optical matrix elements calculated from the above expresion and summarized in table 1 are crude but indicate that the direct optical transitions of $Ge_6/Si_4$ and $Ge_7/Si_3$ are not significant as far as photonics is concerned. For the light polarized along the superlattice axis (perpendicular polarization), all optical matrix elements of $Ge_6/Si_4$ and $Ge_7/Si_3$ are negligible except for the transition from the highest valance band to the second lowest conduction band state ($E_{v1} \rightarrow E_{c2}$) at the centre of BZ. In the case of in-plane polarized light, the optical matrix elements for the

transition from the highest valance band to the lowest conduction band state ($E_{v1} \rightarrow E_{c1}$) at the centre of the BZ are also negligible. In $Ge_7/Si_3$ strained superlattices only transitions from the second and third valance band to the lowest conduction band state ($E_{v2} \rightarrow E_{c1}$ and $E_{v3} \rightarrow E_{c1}$) have non-zero optical matrix elements. For $Ge_6/Si_4$ system, transitions from second and third valance band states to the second conduction band state ($E_{v2} \rightarrow E_{c2}$) and $E_{v2} \rightarrow E_{c3}$) have small but finite optical matrix element at the zone centre.

In conclusion, both $Ge_6/Si_4$ and $Ge_7/Si_3$ strained superlattices have direct band gaps but optical matrix elements for corresponding transitions are negligible. This is in agreement with experiment, which fails to observe these transitions. Possible direct transitions are from the second and third valance band states to the first (for $Ge_7/Si_3$) and to the second (for $Ge_6/Si_4$) conduction band states.

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